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**FIRST COMPUTER CODE FOR PREDICTING
THERMOCHEMICAL EROSION IN GUN BARRELS**

**SAMUEL SOPOK
PETER O'HARA
GEORGE PFLEGL
STUART DUNN
DOUGLAS COATS**

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DEVELOPMENT AND ENGINEERING CENTER
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BENÉT LABORATORIES
WATERVLIET, N.Y. 12189-4050**



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13. ABSTRACT (Maximum 200 words) An update is provided for the previously-presented gun barrel thermochemical erosion modeling code. This code addresses wall degradations due to transformations, chemical reactions, and cracking. As a predictive tool, it provides analysis and design information that is either unattainable or expensive by experiment. Single- or multiple-shot comparisons can be made of either the same gun wall material for different rounds, or different gun wall materials for the same round. This complex computer analysis is based on rigorous scientific thermochemical erosion considerations that have been validated in the reentry nosetip and rocket nozzle/chamber community over the last forty years. A gun system example is used to illustrate the five module analyses for chromium and gun steel wall materials for the same round. The first two modules include the somewhat modified standard gun community XNOVAKTC interior ballistics and BLAKE nonideal gas thermochemical equilibrium codes. The last three modules, significantly modified for gun barrels, include the standard rocket community two-dimensional kinetics/mass addition boundary layer (TDK/MABL), gas-wall thermochemistry (TDK/CET), and wall material ablation conduction erosion (MACE) codes. These five analyses provide thermochemical ablation, conduction, and erosion profiles for each material as a function of time, travel, and rounds. For the gun system example, at two axial positions, with cold and hot firing rates, predictions of rounds required to achieve 0.040-inch wall loss are made for cracked and uncracked 0.005-inch chromium plated A723 steel and A723 steel alone. Thermochemical erosion increases by a factor of about 2.0 from cracked chromium plated A723 steel to A723 steel alone. For a given wall, thermochemical erosion decreases by a factor of 1.4 from the hot to the cold firing rates. Since uncracked chromium plated A723 steel is virtually uneroded, it appears that A723 steel ablation at the chromium cracks leaves unsupported chromium, which is subsequently removed by the high-speed gas flow. These predictions agree well with actual gun system erosion data. Thermochemical ablation is supported by actual gun system materials analyses, which provided no evidence of melt-type ablation.				
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INTRODUCTION

Aerothermochemistry is the study of chemical reactions in flow systems and was first described by von Karman in 1951 (ref 1). The modification of the heat transfer coefficient by a blocking effect for the mass addition of chemically reacting wall material into the boundary layer was first described by Reshotko and Cohen in 1955 (ref 2) and Cohen et al. in 1957 (ref 3). The thermochemical erosion of reentry vehicle (RV) heat shield material for various chemically reacting systems was first studied by Denison and Dooley in 1957 (ref 4).

Denison and Dooley's thermochemical erosion analysis regarding convective heat transfer with mass addition and chemical reactions was subsequently unified and summarized by Lees of California Institute of Technology (consultant to the Ramo-Wooldridge Corporation) in 1958 (ref 5). From early thermochemical erosion models, to JANNAF standardized current models (refs 6,7), the near exclusive use of Lees' analysis has stood the test of time, and demonstrates that the major assumptions in his 1958 paper are still reasonable and valid for RV nosetips and rocket chambers/nozzles.

In the last twenty years, gun barrel technology has primarily focused on mechanical and metallurgical aspects with a secondary focus on erosion. Catastrophic gun barrel failures have been nearly eliminated, while thermochemical erosion (thermochemical ablation with mechanical erosion) problems have intensified due to performance requirements demanding the use of high-flame temperature propellants. The erosion of gun barrels is generally attributed to both thermal ablation (bore surface phase transformations with aerodynamic flow removal) and thermochemical ablation (gas-wall chemical reactions with aerodynamic flow removal), although the surface temperature should remain below the solidus temperature for a practical gun design.

In 1990, the U.S. Army Benet Laboratories (Benet) conducted an extensive literature search of military, NASA, and commercial sources that revealed no "shrink-wrapped" thermochemical erosion modeling codes for gun barrels. This search did reveal the JANNAF standardized rocket community counterpart, which includes the two-dimensional kinetics (TDK) (chemistry by CET and mass addition boundary layer (MABL)), as well as the materials ablation conduction erosion (MACE) modeling codes for predicting thermochemical erosion for rocket chambers, nozzles, and nosetips (refs 6-8). Software and Engineering Associates, Inc. (SEA) is now the sole maintainer and developer of the TDK/MACE rocket erosion codes.

In 1991, Benet and SEA mutually determined that these rocket codes should be modified for guns and that these codes actually exceeded gun erosion code requirements and expectations (ref 9). It became obvious that two of the analytical tools needed to begin the thermochemical erosion analysis of gun barrels were already available in the gun community. These tools were Freedman's BLAKE thermodynamic equilibrium code with compressibility (ref 10), and Gough's NOVA interior ballistics code (ref 11). SEA and Benet successfully modified the BLAKE, NOVA, TDK, and MACE codes into what appears to be the first unified gun erosion code (ref 9).

A joint SEA/Benet research seminar was given at Benet on this first unified gun erosion code to present its capabilities, using a gun system example where erosion cannot be explained by thermomechanical effects alone (refs 9,12). Several JANNAF-sponsored gun erosion meetings have implied a gun system-specific thermochemical erosion component for many previous gun systems (ref 13). For this gun system example, with its solid propellant product-steel (or chromium plated steel), an ablative scale-like oxidation of iron and chromium by gas-wall diffusion of oxygen predominates, and these loosely held crack-rich brittle scale layers are easily removed by mechanical erosive forces. U.S. Army experimental data support the existence of gun barrel oxidation (ref 14). In July 1995, the first-known gun barrel thermochemical ablation-mechanical erosion modeling code was published by Benet (ref 15), and a summary is presented in this report. In October 1995, the Army Research Laboratory (ARL) published its thermal ablation-mechanical erosion gun modeling code (ref 16) and has not published the addition of a chemical component to date.

PROCEDURE

The thermochemical erosion analysis procedure for the 155-mm unicannon gun system (ref 12) (full charge) consists of five analyses, including the following codes:

- NOVA (refs 9,11) (interior ballistics and core flow)
- BLAKE (refs 9,10) (gas thermochemistry and compressibility)
- TDK/MABL (refs 6,9) (heat transfer modified by boundary layer mass addition, decoupled from core flow)
- TDK/CET (refs 6,8-9) (gas-wall thermochemistry)
- MACE (refs 7,9) (ablation, conduction, and erosion profiles)

The TDK/MABL module generates transport properties, Mollier gas properties, adiabatic conditions, and cold wall heat transfer conditions using NOVA/BLAKE data as input. The TDK/CET module generates H-B Mollier chart linkage files for nonreacting (inert) walls, reacting chromium walls, and reacting A723 steel walls using NOVA/BLAKE data as input; combustion product omissions are based on experimental testing and a U.S. Army report (ref 14). The MACE code calculates the transient thermochemical response and generates ablation, conduction, erosion surface, and depth profiles as a function of time, travel, and rounds. MACE uses NOVA, BLAKE, MABL, and CET data as input for the cracked and uncracked 0.005-inch chromium plated A723 steel and A723 steel alone walls at two axial locations (1 and 2 feet) and two firing rates (cold single shot and hot 12 rpm bursts). MACE gas-wall chemical kinetics data are based on testing and the literature (ref 9).

RESULTS AND DISCUSSION

For this thermochemical erosion analysis, any propellant-wall combination can be modeled, each mechanism's importance is identified, computer resources are modest (high-end PC), parametric analysis is possible, and incremental upgrades are feasible. However, this approach requires engineering judgement and extrapolations are questionable.

The NOVA analysis outputs the pressure, velocity, and temperature core flow as a function of time and travel. The BLAKE analysis outputs pressure-temperature-compressibility data, as well as thermochemistry data.

The TDK/MABL analysis outputs adiabatic wall recovery enthalpy (H_r) and adiabatic wall temperature (T_{aw}) data as a function of time and travel. The recovery enthalpy is the potential chemistry driver where the heat transfer approaches zero and the adiabatic wall temperature is the potential temperature without reactions. The TDK/MABL analysis also outputs cold wall heat transfer rate (Q_{cw}) data as a function of time and travel. This heat transfer rate is the wall heat flux evaluated at the cold wall temperature.

The TDK/MABL heat and mass transfer model includes the following three equations. The first equation is for mass addition to the boundary layer, the second equation is for heat-to-mass transfer ratio, and the third equation is for the overall correlation between the first and second equations:

$$r_e U_e Ch_o = Q_{cw} / (H_r - H_{gw}) \quad (1)$$

$$r_e U_e Ch_b = Mdot_g / B_a; Le = 1 \quad (2)$$

$$Ch_b / Ch_o = f(B_a, M_w) = 1 - (h Mdot_g / r_e U_e Ch_o) \quad (3)$$

where r_e is edge density, U_e is edge velocity, Ch_o is Stanton number without blowing, Q_{cw} is cold wall heat transfer, H_r is recovery enthalpy, H_{gw} is gas-wall enthalpy, Ch_b is Stanton number with blowing, $Mdot_g$ is gas mass transfer, Le is the Lewis number, B_a is ablation potential, M_w is molecular weight, $h = a(M_{we}/M_{wi})^{**b}$, h is related to the molecular diffusion of the gas into the boundary layer, M_{we} is the molecular weight of the inviscid core at the edge of the boundary layer, M_{wi} is the molecular weight of the injected gas, a is the coefficient, and b is the exponent (ref 9).

The TDK/CET analysis outputs inert gas-wall enthalpy and reacting gas-wall enthalpy (both H_{gw}) data as a function of pressure and temperature for chromium and A723 steel. This analysis also outputs condensed phase mass fraction (C_{cg}) and ablation potential (B_a) data as a function of pressure and temperature for chromium and A723 steel. Choosing chemical equilibrium species requires considerable experience, since they may not actually exist due to kinetic blocking. These products are confirmed by experimental gas-wall analyses for metal combustion products and other applicable literature data (ref 9).

The TDK/CET thermochemical gas-wall analysis is a practical approximation of the gun barrel bore surface due to sufficient combustion gas activation energy (high temperature) and collisions (high pressure) needed for fast gas-wall reaction rates. The TDK/CET ablation model assumes that as the gas diffuses to the wall, it reacts to form products as follows:

$$B_a = (C_w - C_{cg})/C_g = (C_{pg} - C_g)/C_g \quad (4)$$

where B_a is the ablation potential, C_w is the mass fraction of wall material, C_g is the mass fraction of the gas edge, C_{cg} is the mass fraction of condensed phase products, and C_{pg} is the mass fraction of product gas (ref 9).

Figure 1 plots experimental system-specific gas-wall kinetic rate data, normalized mass fraction versus temperature, from a thermogravimetric analysis of the gas-chromium and gas-A723 steel couples needed for MACE code input. Notable features include the gas-wall reaction-limited temperature (T_r) and gas-wall diffusion-limited temperature (T_d) (ref 9). T_r is about 1500°R for A723 steel and 2100°R for chromium. Figure 2 plots experimental material-specific wall softening data, normalized hardness versus temperature, from a thermomechanical analysis of these materials needed for MACE code input. Notable features include the transformation temperature (T_t) of about 1800°R and melt temperature (T_m) of about 3200°R for A723 steel; no T_r , but T_m is about 3800°R for chromium.

The MACE code calculates the actual thermochemical response including wall ablation, conduction, and erosion using the output of the above analyses and experimental or literature gas-wall kinetic rate data. Figure 3 plots MACE analysis outputs of wall temperature (T_w) data as a function of time at two axial positions (1 foot, 2 feet) and two firing rates (1r = cold single shot, 12rb/1m = 12 rpm burst) for chromium and A723 steel. Notable features predict the 1.3 times higher peaked, shorter duration chromium T_w s compared to A723 steel due to A723 steel's higher ablative boundary layer thickening and lower thermal conductivity. For a given wall, other features predict a 150 to 200°R decrease from the 1- to 2-foot axial position and a 90 to 110°R increase from the cold single round to the hot 12 rpm burst.

For the gun system example, at two axial positions (1 foot, 2 feet), with cold and hot firing rates (1r, 12rb/1m), Figure 4 plots MACE predictions of rounds required to achieve 0.040-inch wall loss ($R_{0.040}$) for cracked (1 percent cracked surface area by metallography) and uncracked 0.005-inch chromium plated A723 steel and A723 steel alone. Thermochemical erosion increases by a factor of about 2.0 from cracked chromium plated A723 steel to A723 steel alone. For a given wall, thermochemical erosion decreases by a factor of 1.4 from the hot to the cold firing rates and substantially decreases from axial position 1 foot to 2 feet. Since uncracked chromium plated A723 steel is virtually uneroded, it appears that A723 steel ablation at the chromium cracks leaves unsupported chromium, which is subsequently removed by the high-speed gas flow. For the six eroded wall combinations mentioned, Figure 3 T_w s applied to Figures 1 and 2 show gas-wall reactions and cracking predominate since each of the six combinations

exceeded their T_s s, but none approached their T_m s. These predictions agree well with actual gun system erosion data. Thermochemical ablation is supported by actual gun system materials analyses, which provided no evidence of melt-type ablation.

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Fig 1 - Gas-Wall Kinetic Rate

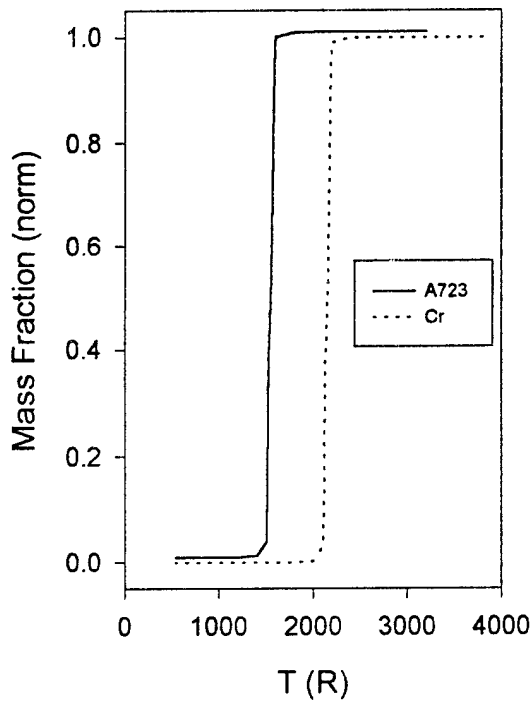


Fig 2 - Wall Softening

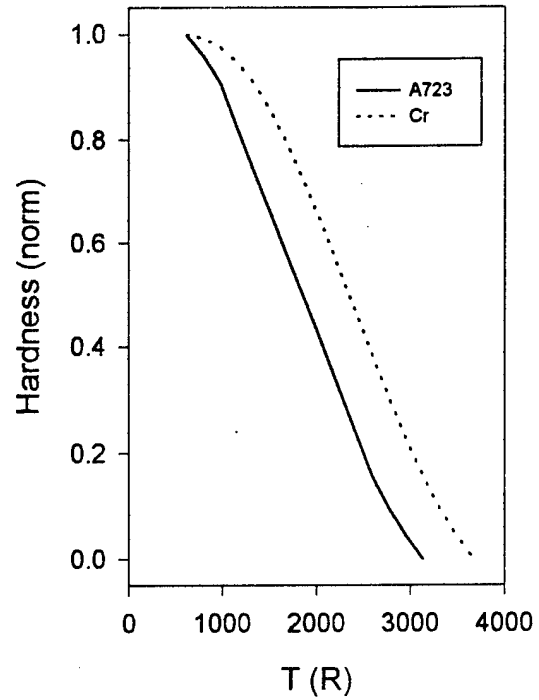


Fig 3 - Wall Temperature

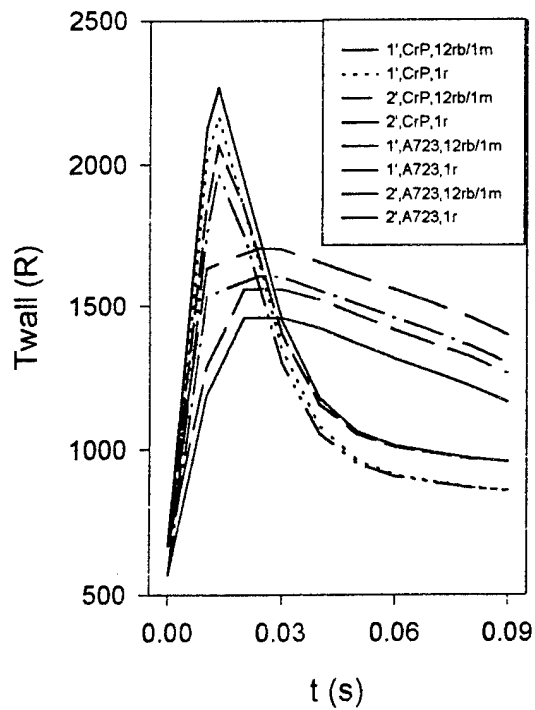
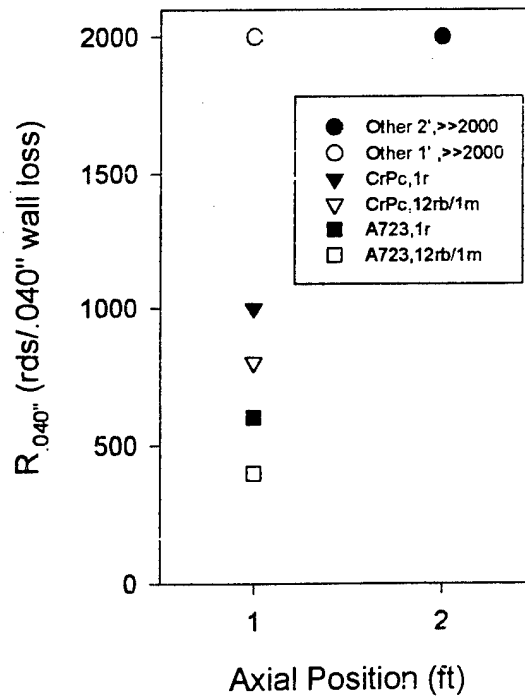


Fig 4 - Rds / 0.040" Wall Loss



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